

Theoretical mechanisms to the control structure and morphology of 2D & 1D materials

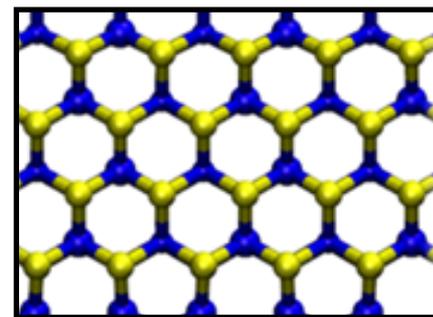
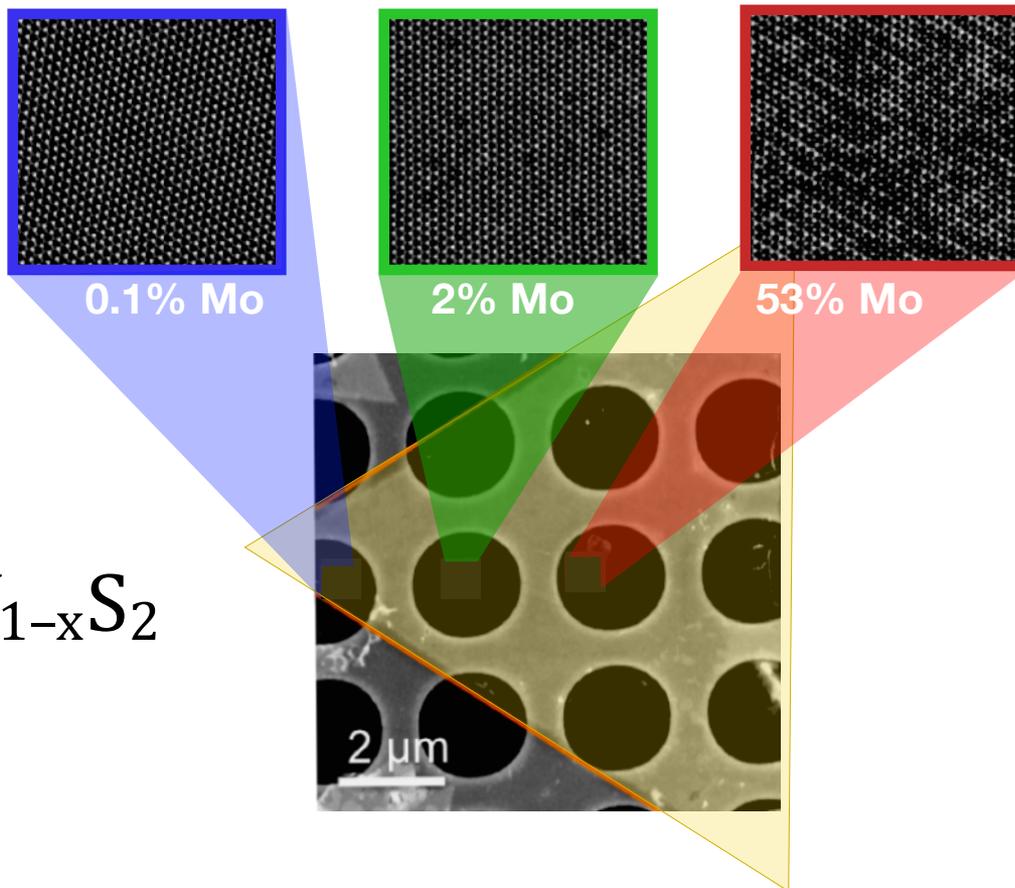
Vincent Crespi



$$2 + 1 = 3$$

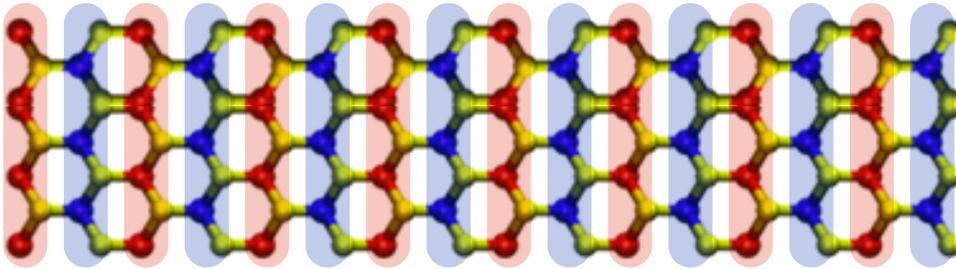


beyond stacking...

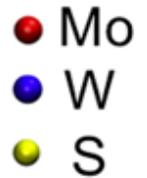
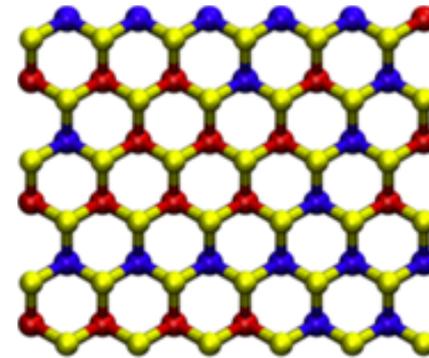


It's not thermodynamics

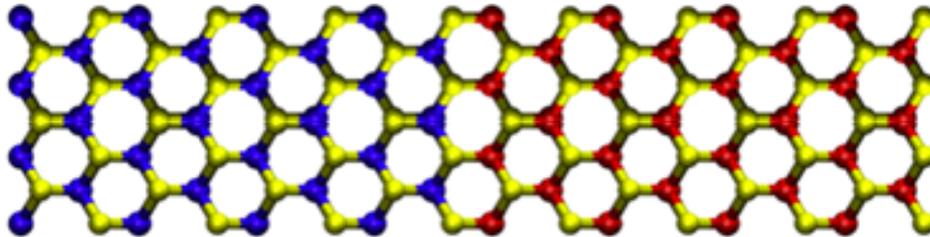
Bulk Stripes



Random Alloy

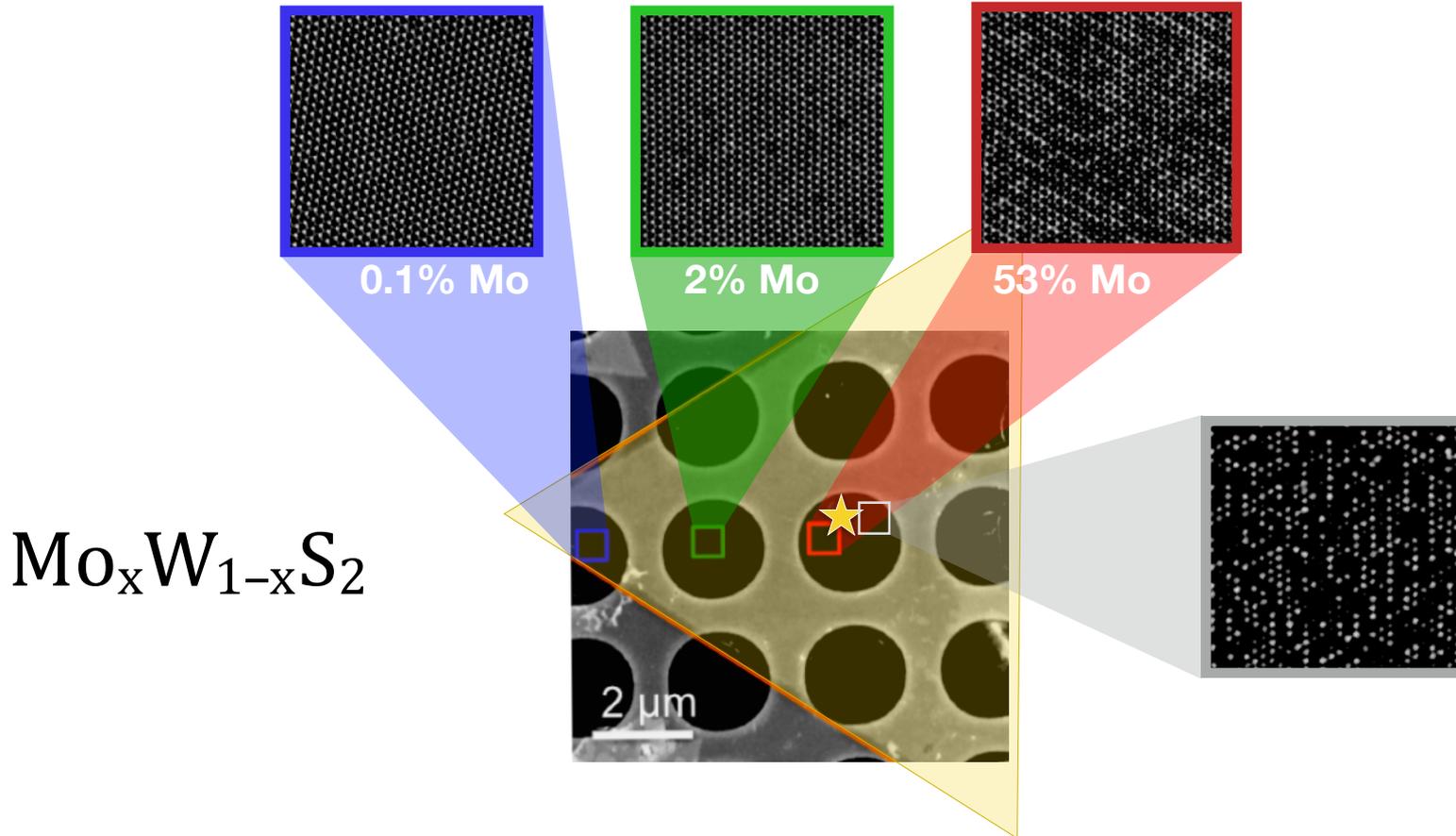


Phase Separation

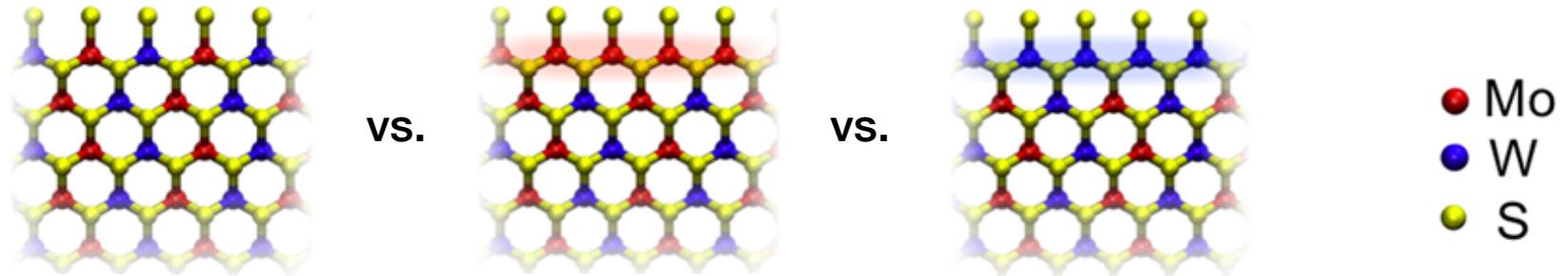


The energy differences between these systems are negligible compared to the growth temperature kT .

What about the other directions?

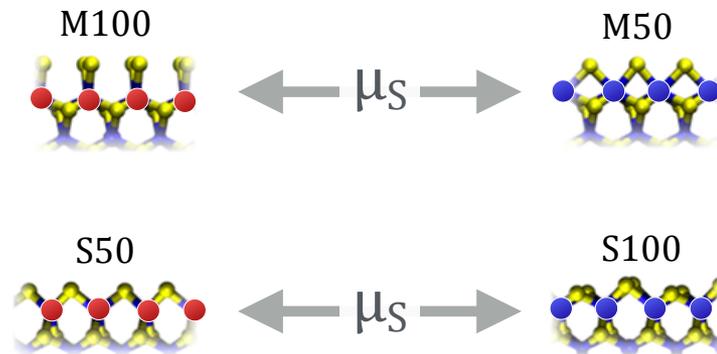


Kinetics, or “Equilibrium of the Edge”



These edges
favor Mo

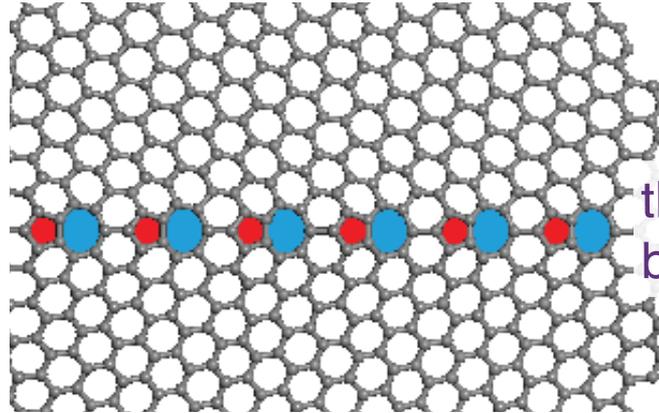
These edges
favor W



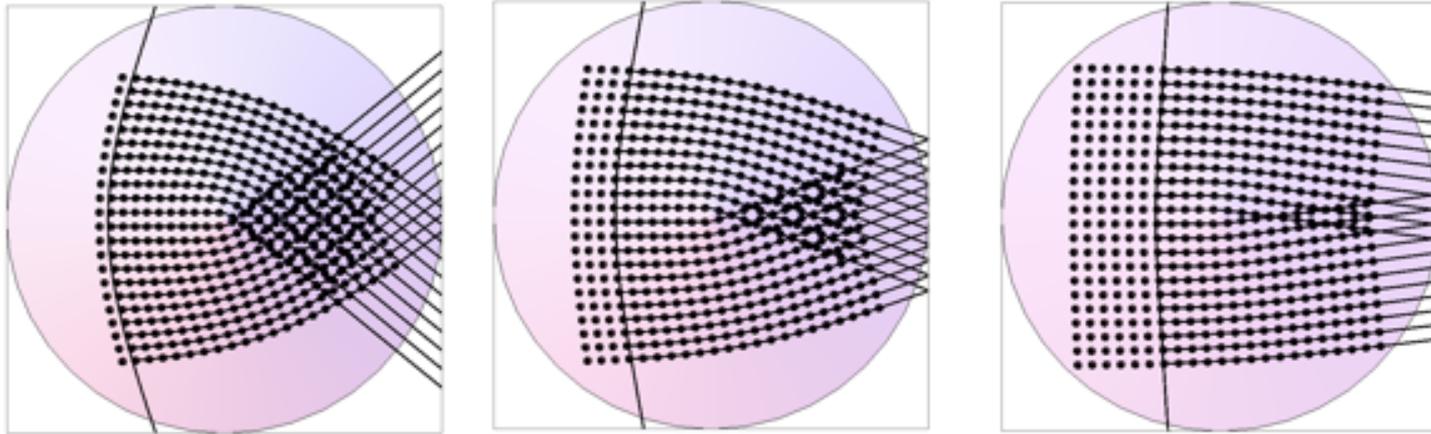
As the sulfur availability fluctuates, the composition of the growth edge alternates, yielding stripes.

Other ways to use the
third dimension?

but it's all one grain!

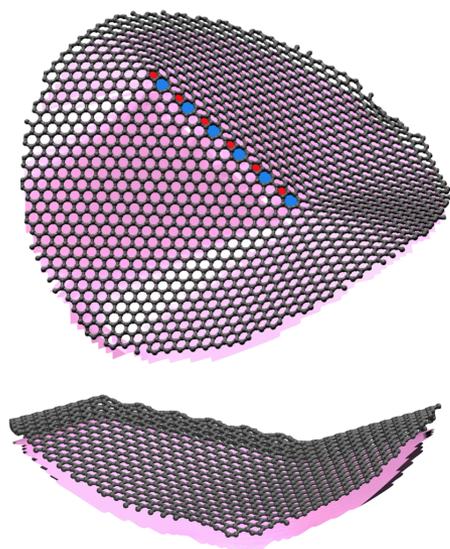


this is a boundary
between two grains

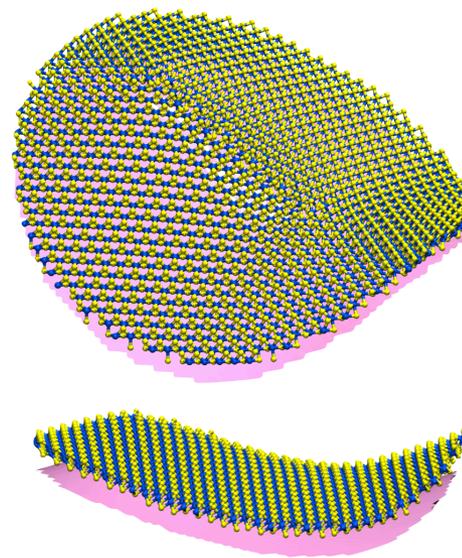


When a growing crystal in two dimensions passes over a bump on the substrate, the growth front self-intersects and we obtain a semi-infinite grain boundary on the “downstream” side.

This grain boundary terminates (or changes angle) at a compensating saddle point.



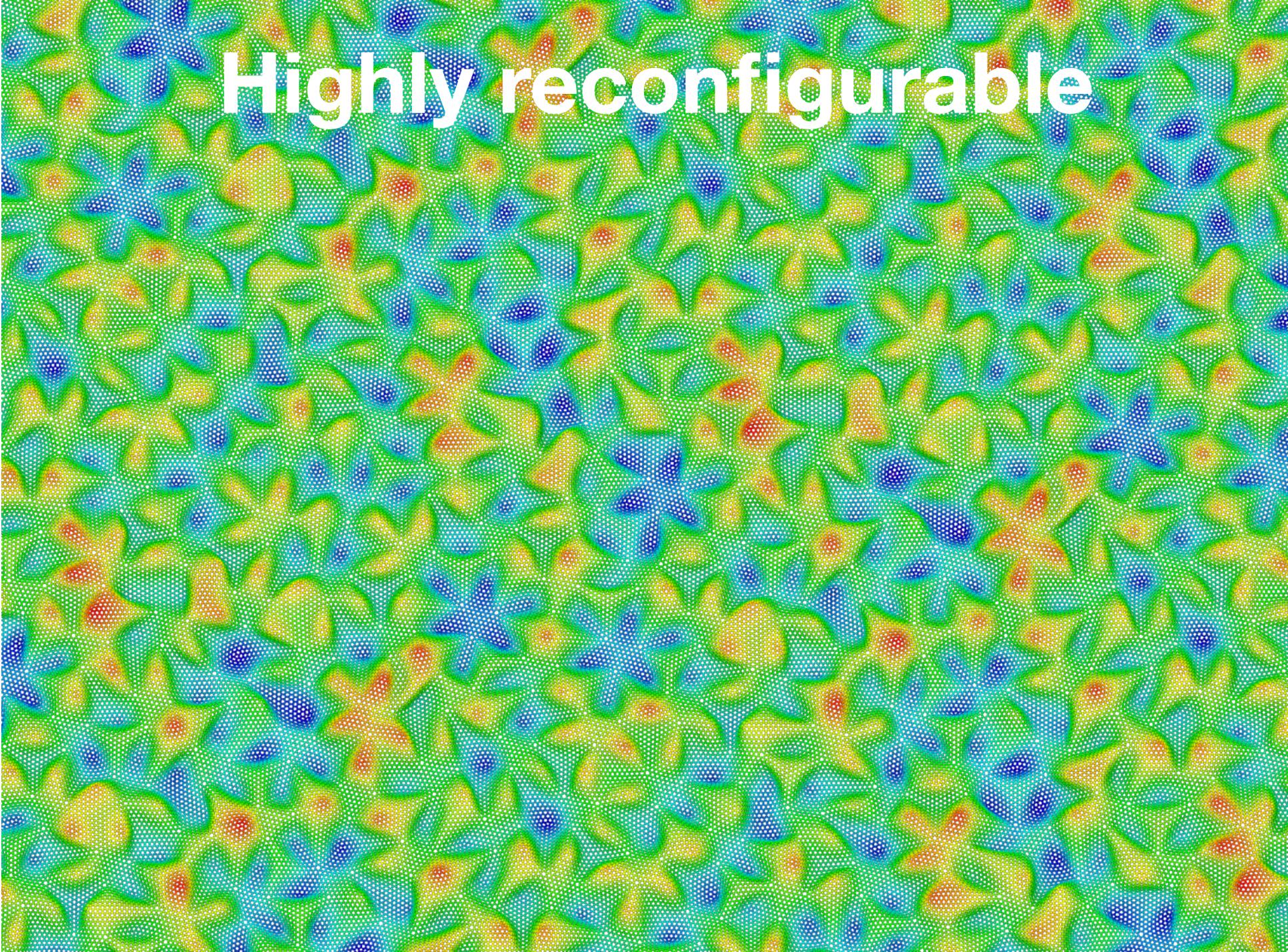
graphene

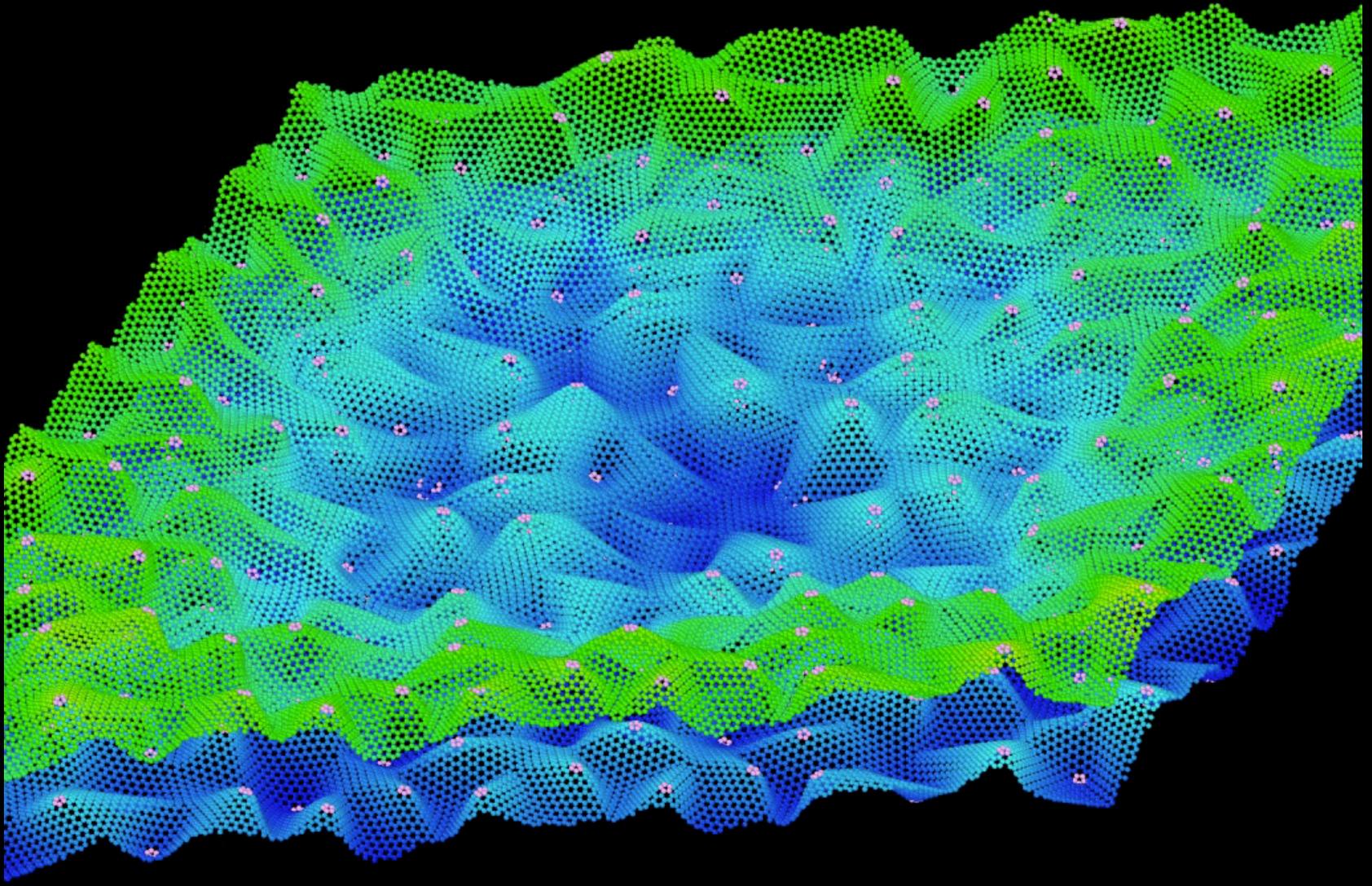


MoS₂

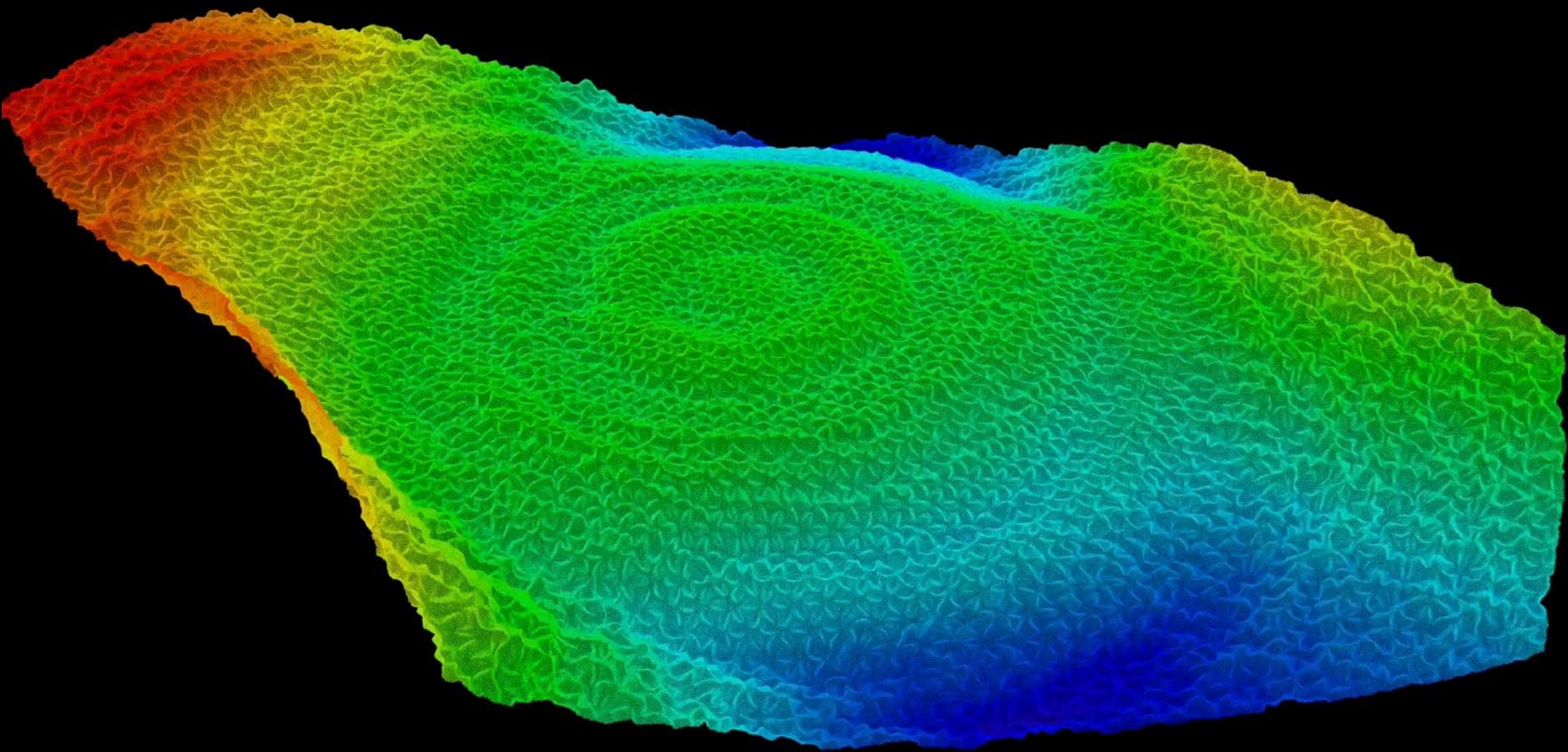
A dense network of grain boundaries of specified angle can be placed at controlled locations by growing on a substrate of designed topography:
Grain boundary materials.

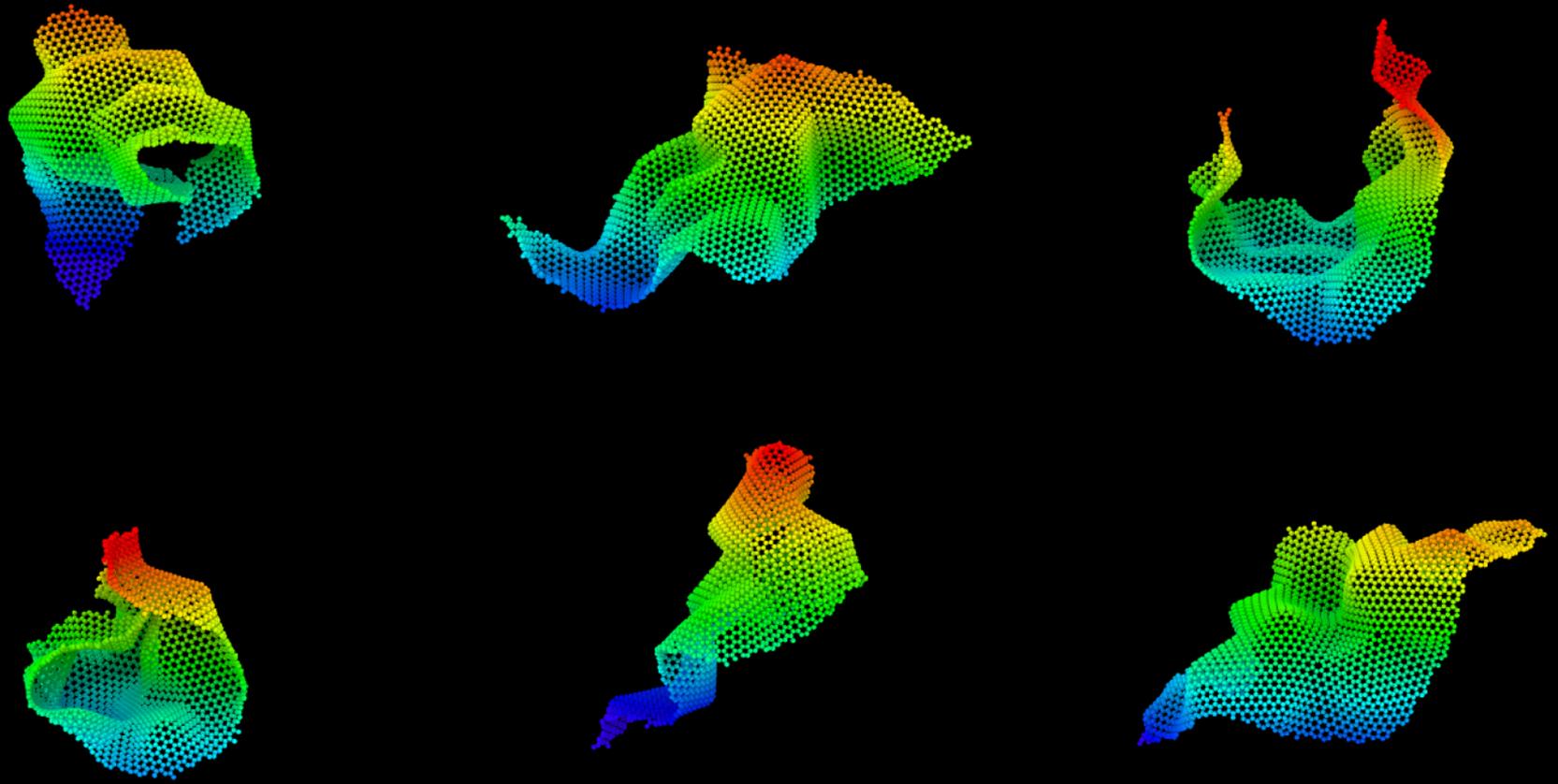
Highly reconfigurable

The background of the slide is a complex, textured pattern. It consists of numerous small, irregular shapes that overlap and interlock, creating a dense, almost crystalline appearance. The color palette is vibrant and multi-colored, featuring shades of green, yellow, orange, and blue. The overall effect is one of a highly reconfigurable and dynamic surface.

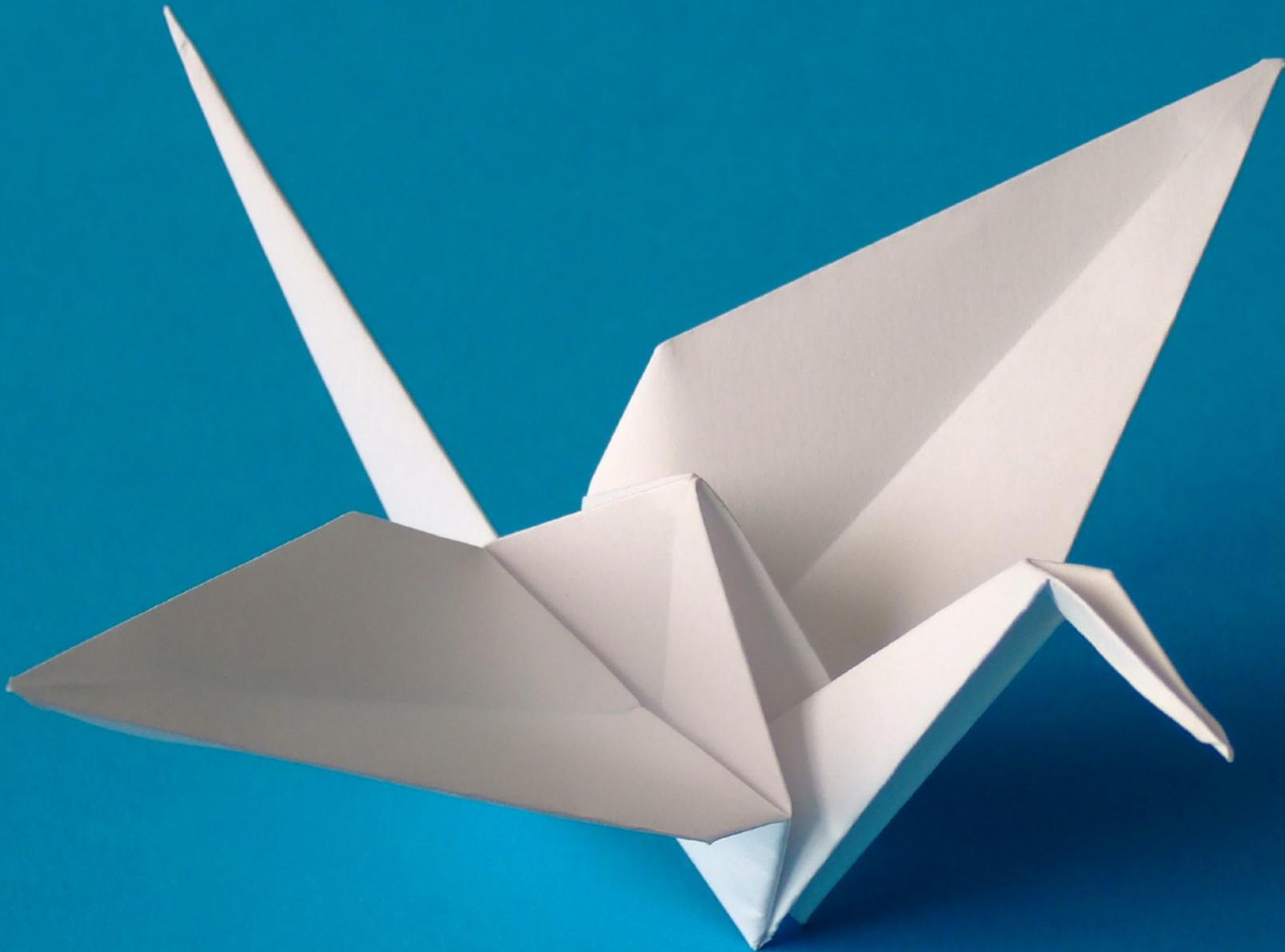


A shape-memory membrane can be lifted off a conformal substrate.

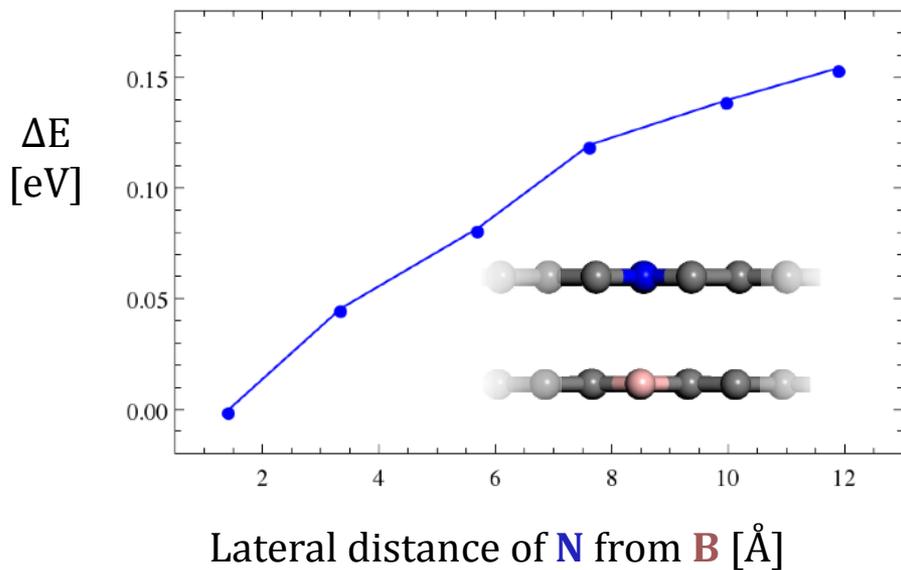
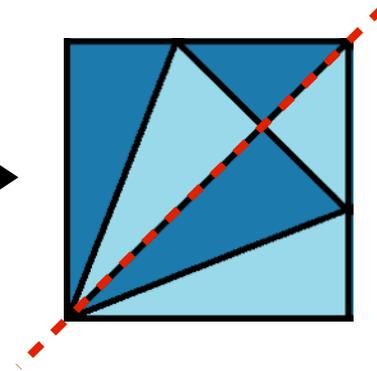
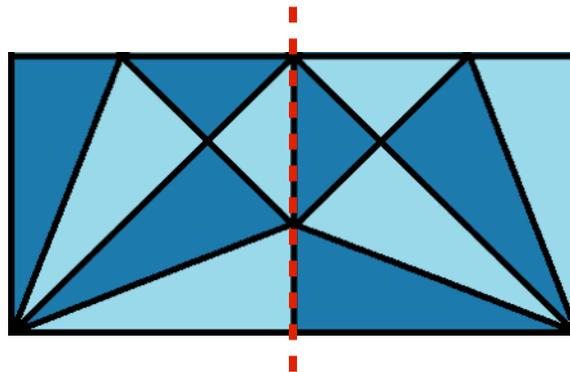
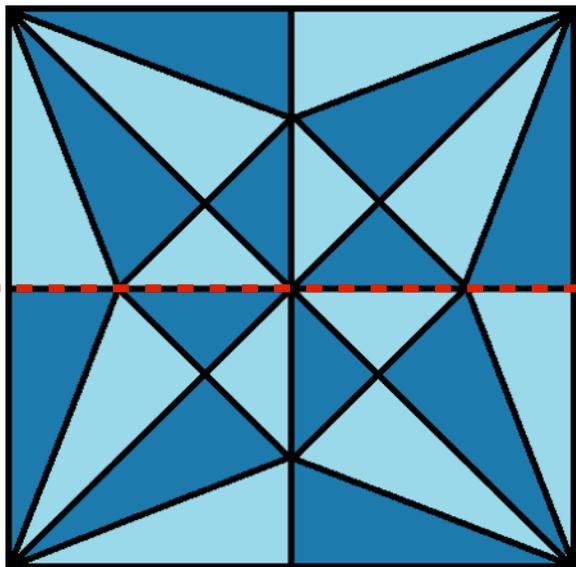


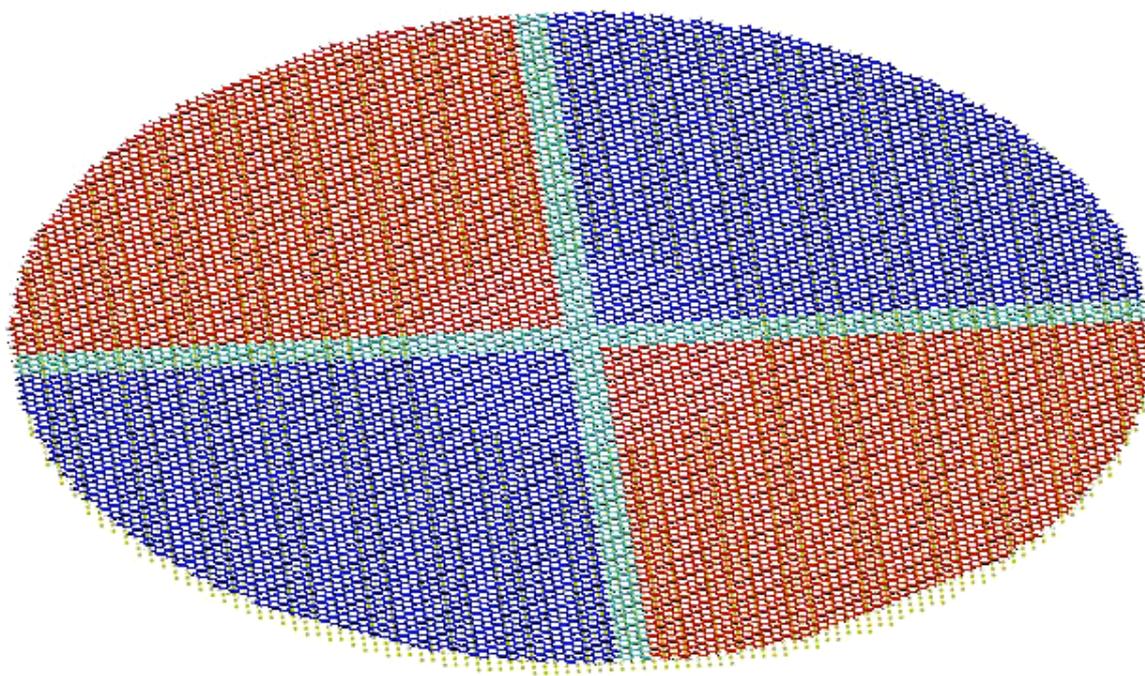


These are different metastable shapes of the *same* membrane. This small piece of membrane has 100's of distinct shapes.



If you fold up a sheet of paper and then flatten it out, you can color the resulting “map” with just two colors.





Yuanxi Wang and V. Crespi, 10.1021/acs.nanolett.7b02773

Grand Challenge

2D will remain a lab curiosity until...

we achieve **wafer-scale, monolayer-controlled growth** of two-dimensional A,B,C,D on top of A,B,C,D with **sufficient quality** that device people are interested.



Grand Challenge

The greatest, most compelling opportunity for a future ground-breaking material system is...

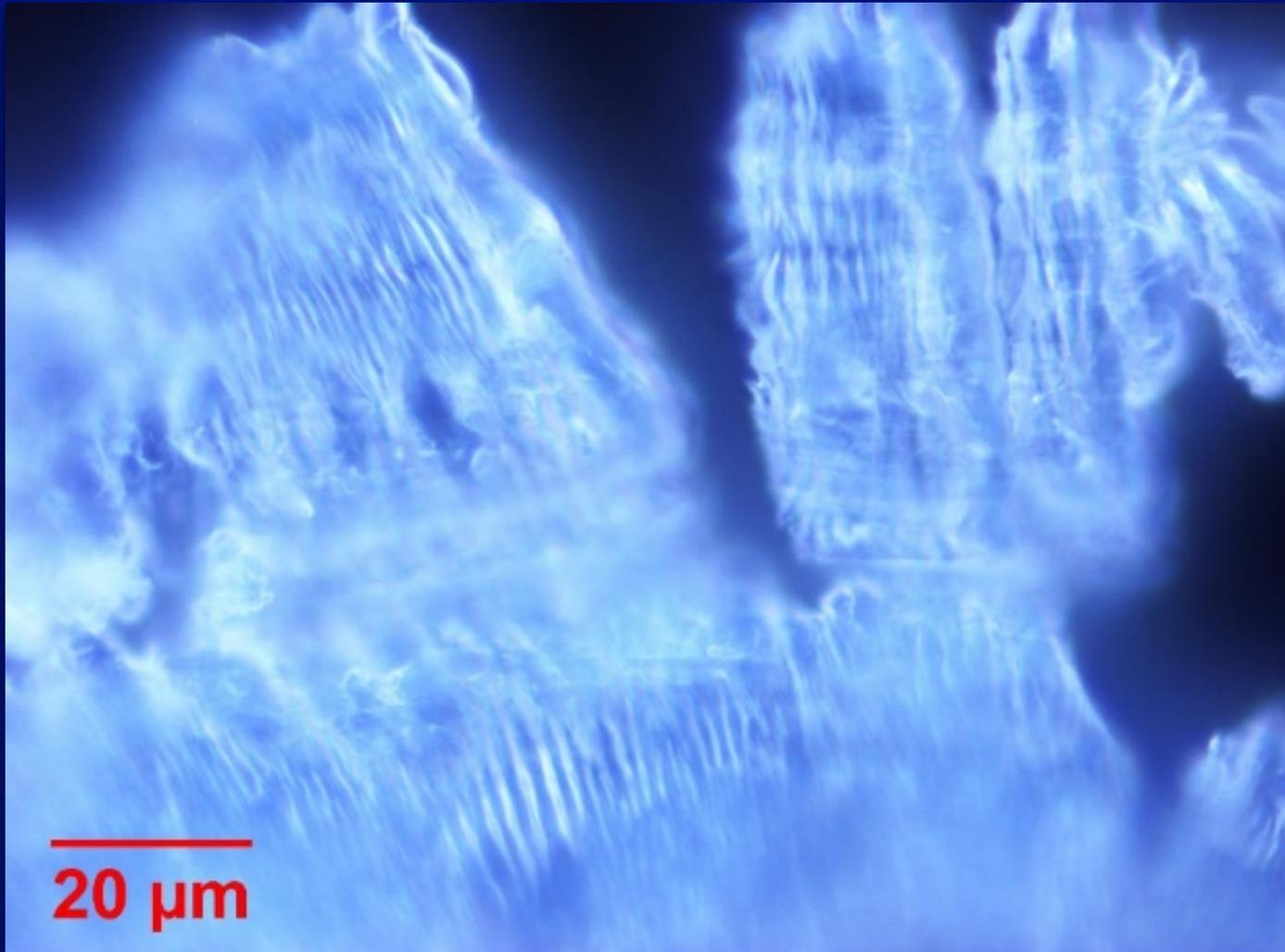
unknown and unknowable

The **grandest challenge** is to design a system of research support that maximizes the rate of new, paradigm-shifting discoveries, which by definition are *outside* any identifiable area of focus.

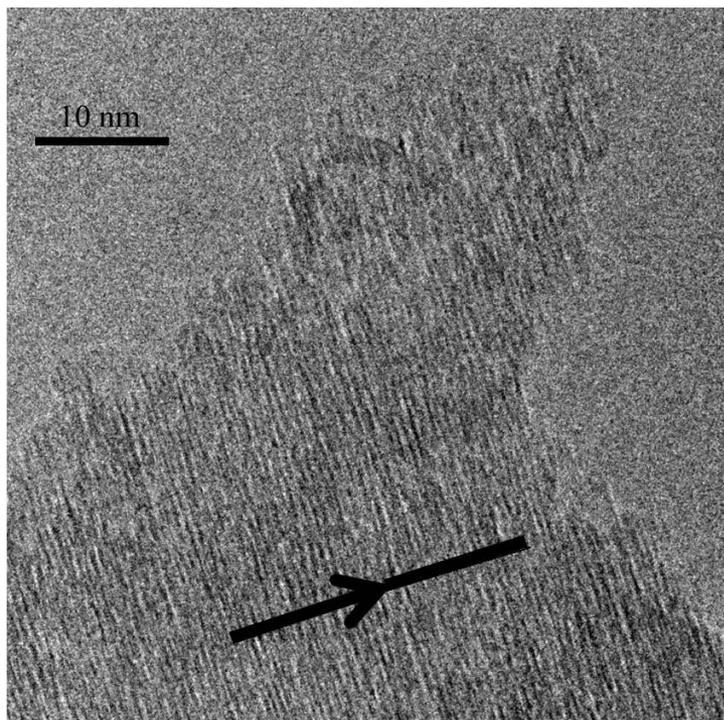
Be true to “transformative”

What is the best mechanism to elicit this sort of activity from the community? Concerted research is important, but at the *fundamental discovery* level we don't want all the antelope grazing from the same patch of grass. Most people are Bosons; we need some of them to be Fermions.

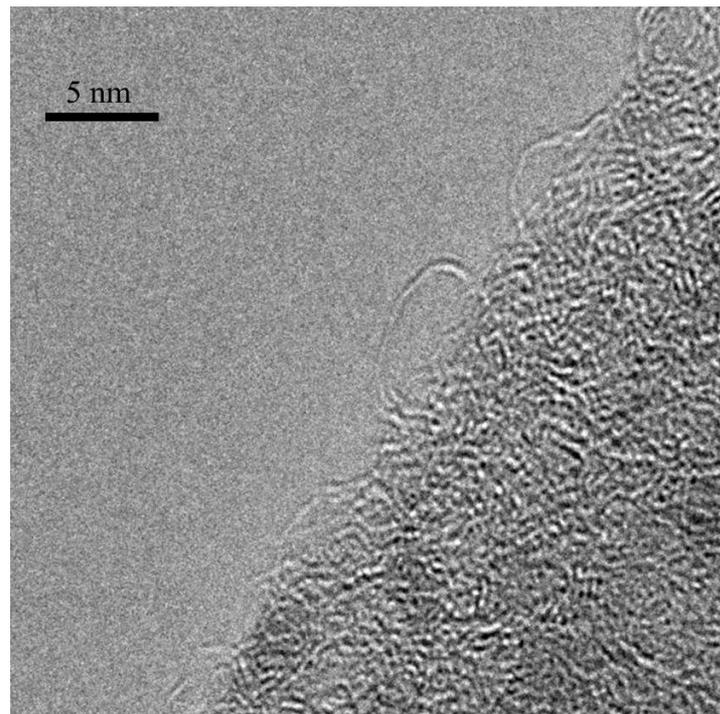
$$1 + 2 = 3$$



as-prepared



after sonication



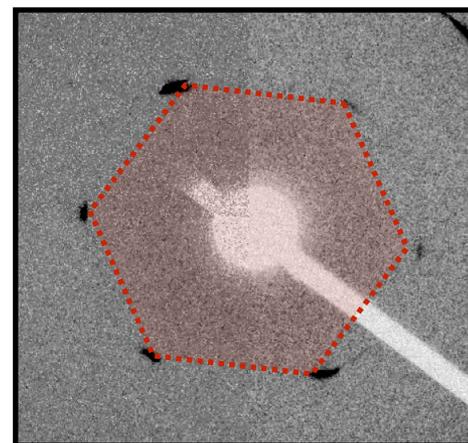
nature
materials

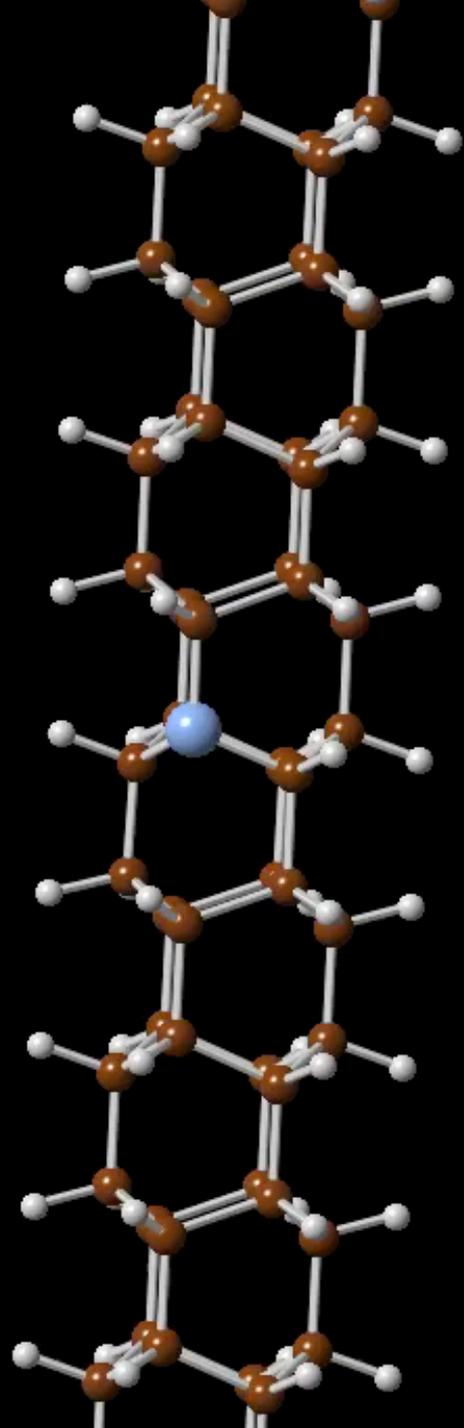
LETTERS

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Benzene-derived carbon nanothreads

Thomas C. Fitzgibbons^{1,2}, Malcolm Guthrie³, En-shi Xu^{2,4}, Vincent H. Crespi^{1,2,4,5},
Stephen K. Davidowski⁶, George D. Cody³, Nasim Alem⁵ and John V. Badding^{1,2*}



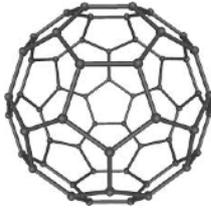


0D

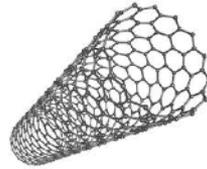
1D

2D

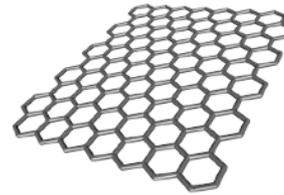
3D



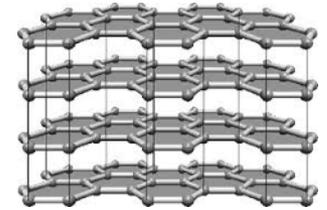
fullerene



nanotube



graphene



graphite

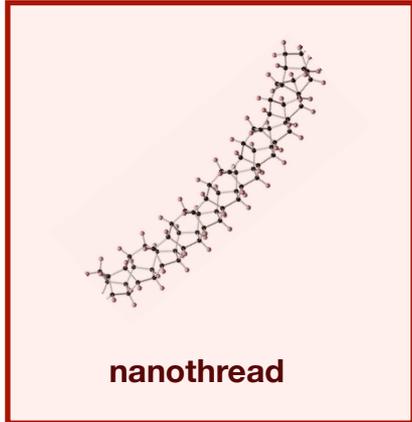
sp^2

Too thick for a polymer : **Stiff enough to be crystalline**

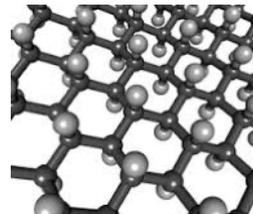
Too thin for a nanowire : **Thin enough to be flexible**



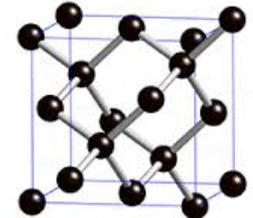
diamondoid



nanothread



graphane



diamond

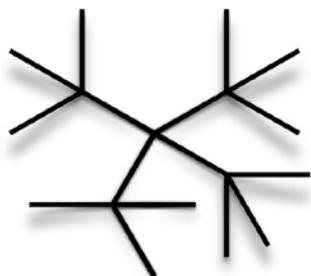
sp^3

Real material properties are determined by nano/micro/meso-structure, not just atomic-scale bonding

This is a new nano/micro/meso-structure for the strongest single bond known.

Periodic boundary
conditions is the great
information destroyer

Numbers of Alkanes (C_nH_{2n+2})

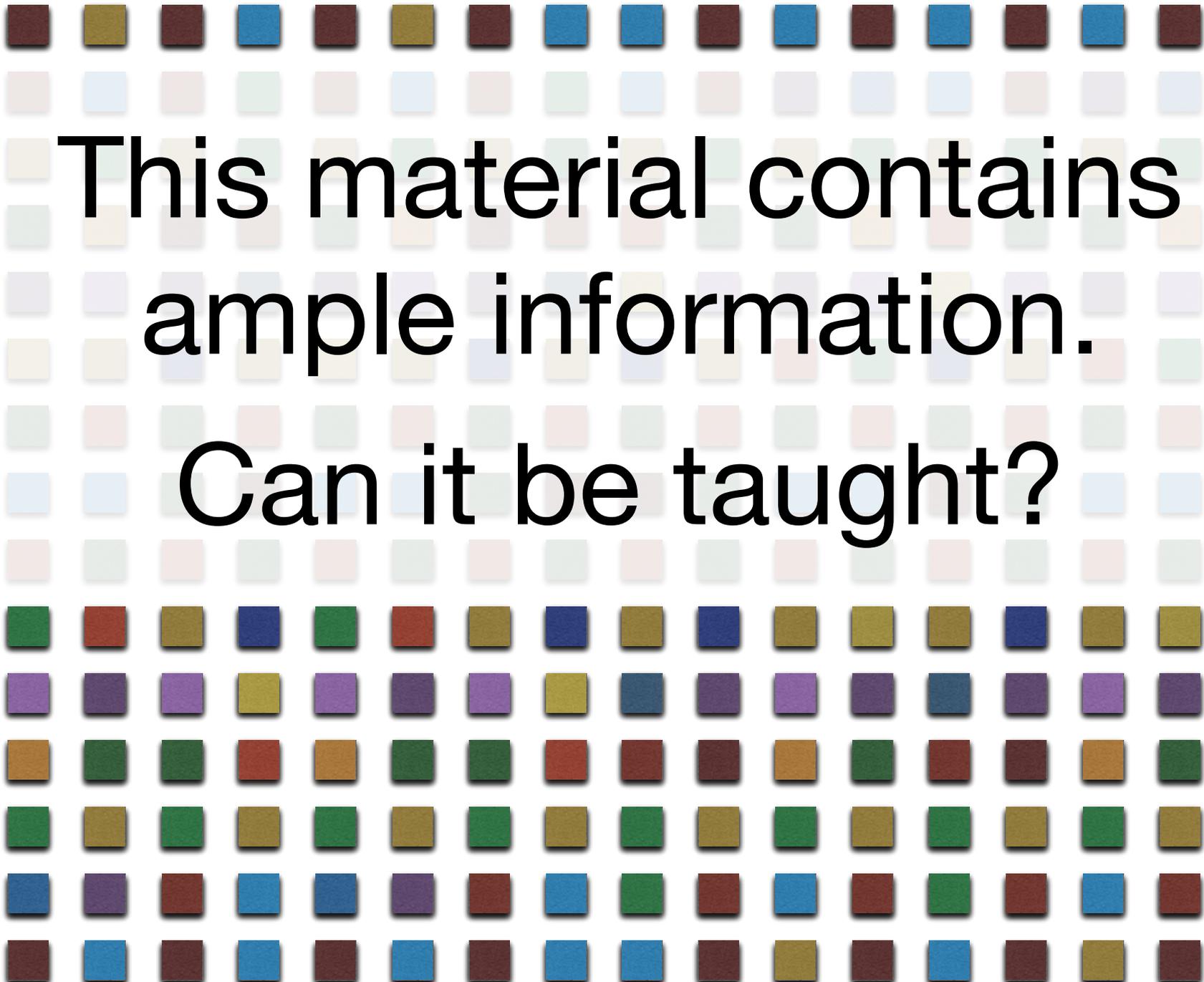


1	1
2	1
3	1
4	2
5	3
6	5
7	11
8	24
9	55
10	136
11	345
12	900
13	2412
14	6563
15	18127
16	50699
17	143255
18	408429
19	1173770
20	3396844
21	9892302
22	28972080
23	85289390
24	252260276
25	749329719
26	2234695030
27	6688893605
28	20089296554

A single modest hydrocarbon has more structures than all equilibrium crystals.

111 260, 135, 156
1 260, 135, 156

Metastable Materials



This material contains
ample information.

Can it be taught?